REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*	2. REPORT TYPE	3. DATES COVERED *(From - To)*
30-08-2011	Briefing Charts	

4. TITLE AND SUBTITLE

Comparison of Reaction Cross Sections for Two DSMC Models and Sensitivity in Non-Equilibrium Flow

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER

6. AUTHOR(S)
Ingrid Wysong, Sergey Gimelshein, Natalia Gimelshein, William McKeon, and Fabrizio Esposito

5d. PROJECT NUMBER

5f. WORK UNIT NUMBER
23080532

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/RZSA
10E. Saturn Blvd.
Edwards AFB CA 93524-7680

8. PERFORMING ORGANIZATION REPORT NUMBER

AFRL-RZ-ED-VG-2011-369

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Air Force Research Laboratory (AFMC)
AFRL/RZS
5 Pollux Drive
Edwards AFB CA 93524-7048

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S NUMBER(S)
AFRL-RZ-ED-VG-2011-369

12. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited (PA #11667).

13. SUPPLEMENTARY NOTES
For presentation at DSMC 11, Santa Fe, NM, 25-28 Sep 2011.

14. ABSTRACT

This is a presentation to DSMC 11 on comparing reaction cross sections for two DSMC models and sensitivity in a non-equilibrium flow.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Andrew D. Ketsdever
Unclassified	**Unclassified**	**Unclassified**	SAR	21	19b. TELEPHONE NUMBER *(include area code)* N/A

AFRL

THE AIR FORCE RESEARCH LABORATORY

LEAD | DISCOVER | DEVELOP | DELIVER

COMPARISON OF REACTION CROSS SECTIONS FOR TWO DSMC MODELS AND SENSITIVITY IN NONEQUILIBRIUM FLOW

Ingrid Wysong, Sergey Gimelshein, Natalia Gimelshein, William McKeon, Fabrizio Esposito

Acknowledgements

- Wysong AFRL
- Gimelshein, Gimelshein, McKeon ERC, AFRL
- Esposito IMIP-CNR, Bari
- Support from the Air Force Office of Scientific Research, Dr. Mitat Birkan program manager, is gratefully acknowledged.

Introduction:
DSMC Chemistry Models

- Important for hypersonic reacting flows (re-entry): strong nonequilibrium, large effect on heating, radiation
- Long history of proposed simplified models; realism can be improved **if** reaction behavior is well understood
- After flurry of work inspired by BSUV data, many felt that without new measurements, further work unfruitful
- New(ish) Quantum Kinetic (QK) model proposed by Bird has generated renewed interest

QK Model

- See G.A. Bird, Gallis, references therein
- Very appealing simplicity
- Impressively predicts thermal rate coefficients k(T) over wide T range in good agreement with measured/recommended values
- The present paper investigates the behavior of $\sigma(E)$, or reaction probability per collision, important for strongly nonequilibrium flows
- Available detailed quasi-classical trajectory (QCT) results for $\sigma(E)$ for 2 important reactions are used to evaluate

Model Definitions

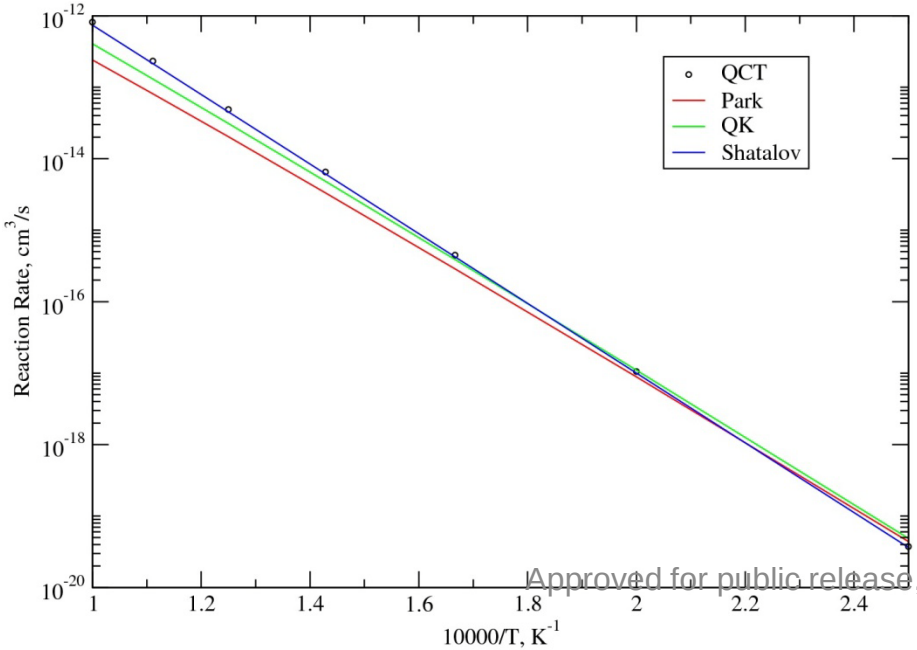
- **QK dissociation: Preact =1 for Ec>Ea, =0 otherwise**
- **QK exchange:**
- **Total Collision Energy (TCE)*: reproduces**
  - $k(T) = AT^{B}\exp(-E_a/T)$ for given values of A, B, E_a and ζ
- **Both models need total collision cross section values: VHS model parameters selected so that collision-pair viscosity matches values predicted by Capitelli (ref) in 5,000 – 15,000K range**
- *** Bird, 1994.**

Vibrational Energy Levels

- Original TCE model used continuous internal energy modes
- Later work adapted it for quantized internal energy levels, see esp Gimelshein (ref) and discussion of small correction factor to use for simple harmonic oscillator (SHO) levels; zero-point vibrational energy (ZPE) is included in total collision energy
- QCT calculations of course use real vibrational energy level values (closer to AHO)
- This work compares DSMC results for SHO levels to QCT results for AHO levels which have same Evib

N_2+N Dissociation Reaction

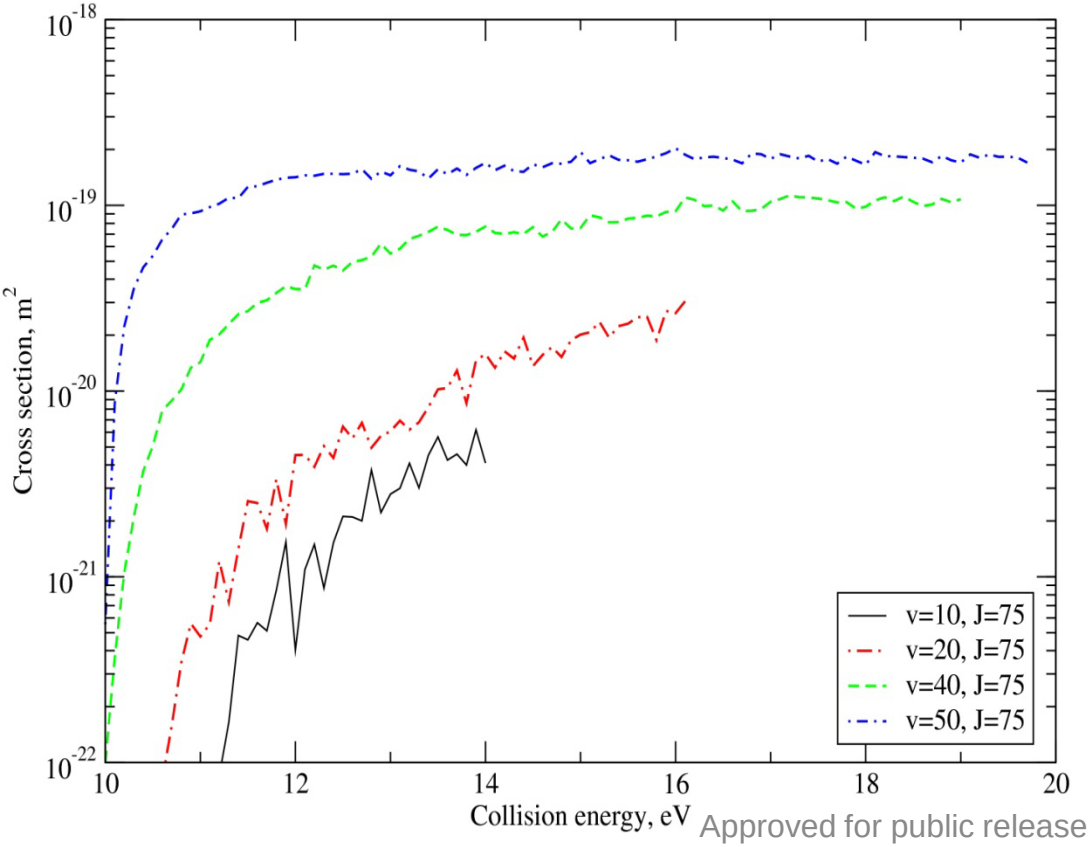
- **Plot of thermal reaction rate coefficients**
- **TCE model uses published Arrhenius parameters as input and will match QCT k(T) by definition**
- **QK model uses no adjustable parameters and matches QCT (and expt) k(T) quite closely**



QCT results from Esposito et al., (**Chem Phys. 331** 2006)

N_2+N Dissociation Reaction

- **QCT σ results from Esposito** (Chem Phys Lett 302, 1999 and unpublished)
- **Dissociation reaction, as is well-known, has strong vibrational favoring**

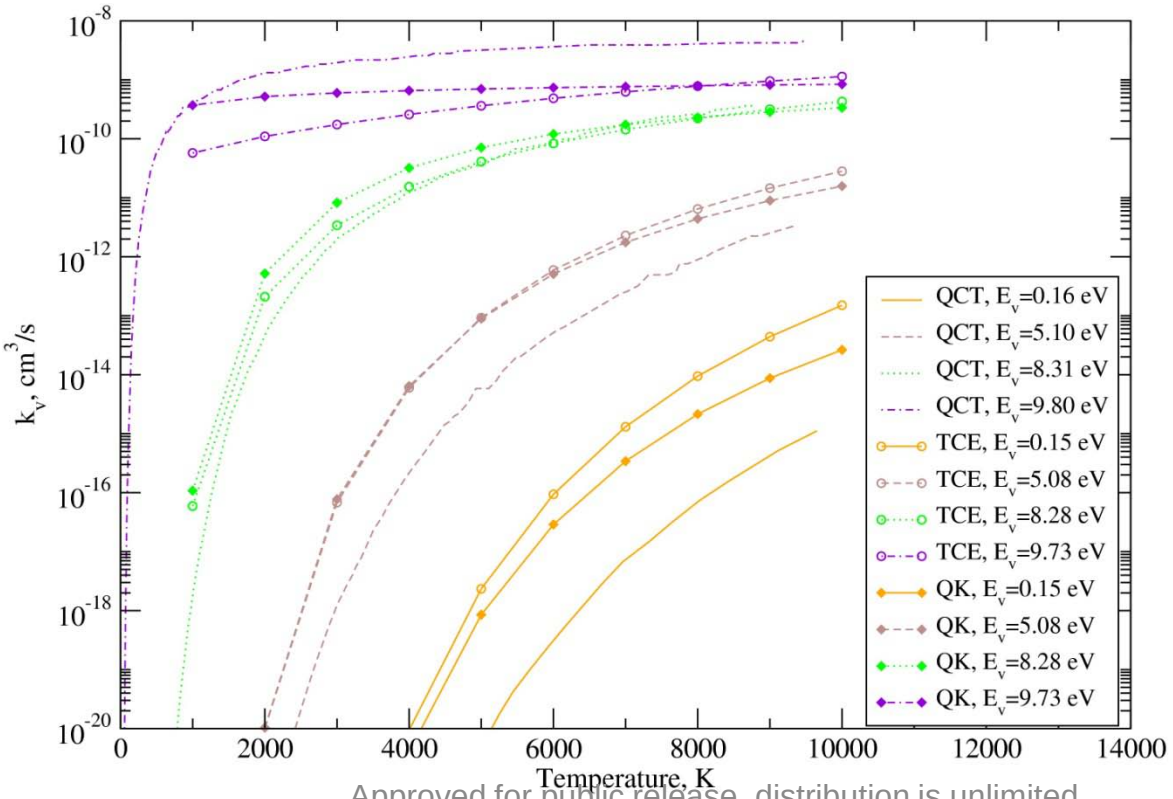


QCT cross sections at same E_c show >100x difference in σ!

No simplified DSMC reaction model includes this effect

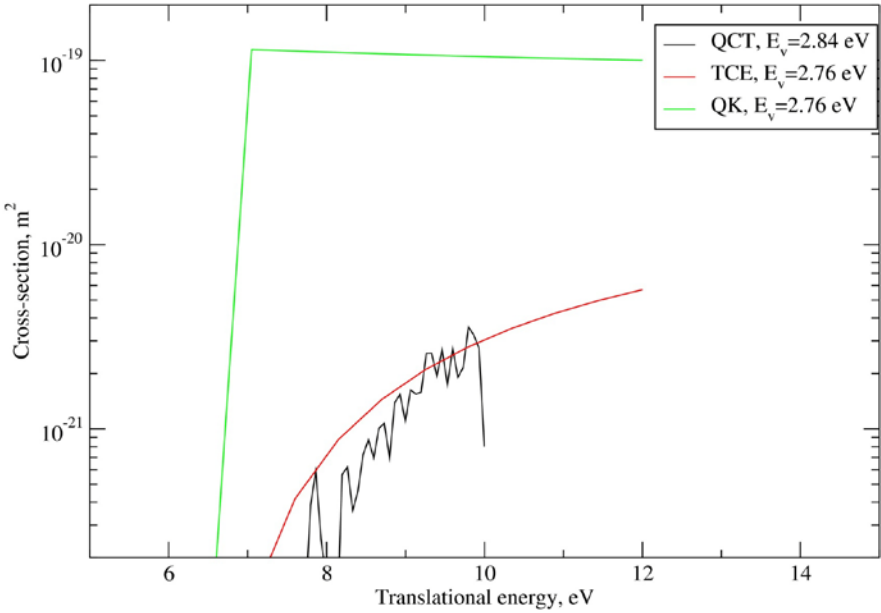
N_2+N Dissociation Reaction

- **State-specific thermal rates $k_v(T)$**
- **TCE and QK models both have $k_v(T)$ that are high for low-v and low for high-v levels. No surprise.**



N_2+N Dissociation Reaction

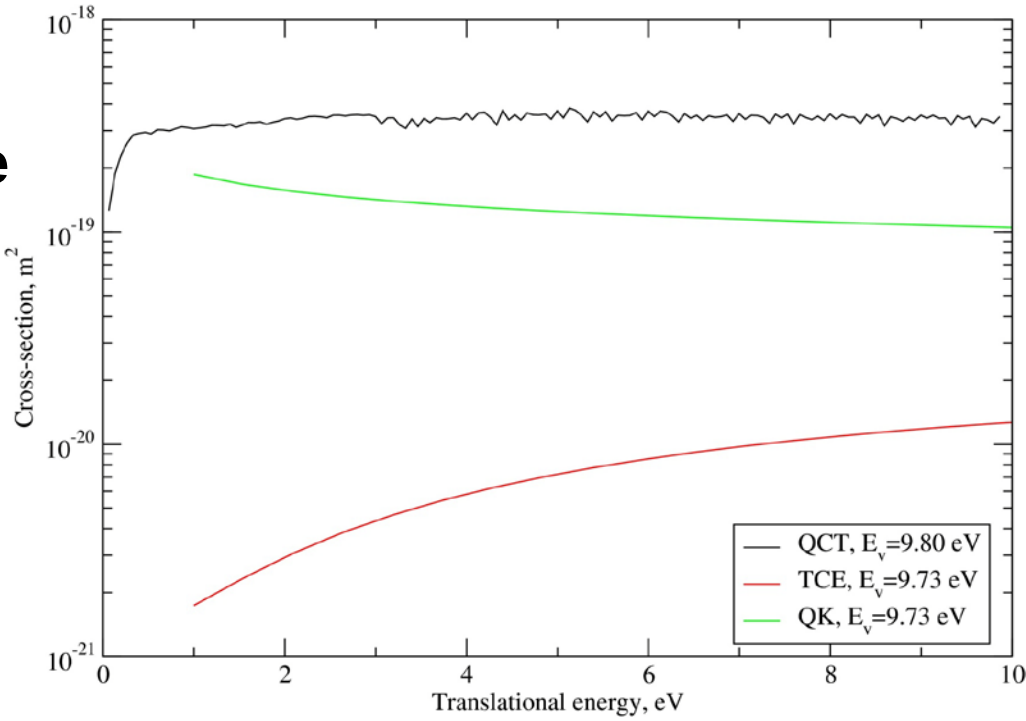
- QK assumes that each collision above threshold energy has unity reaction probability
- TCE matches realistic QCT σ surprisingly closely



N_2+N Dissociation Reaction

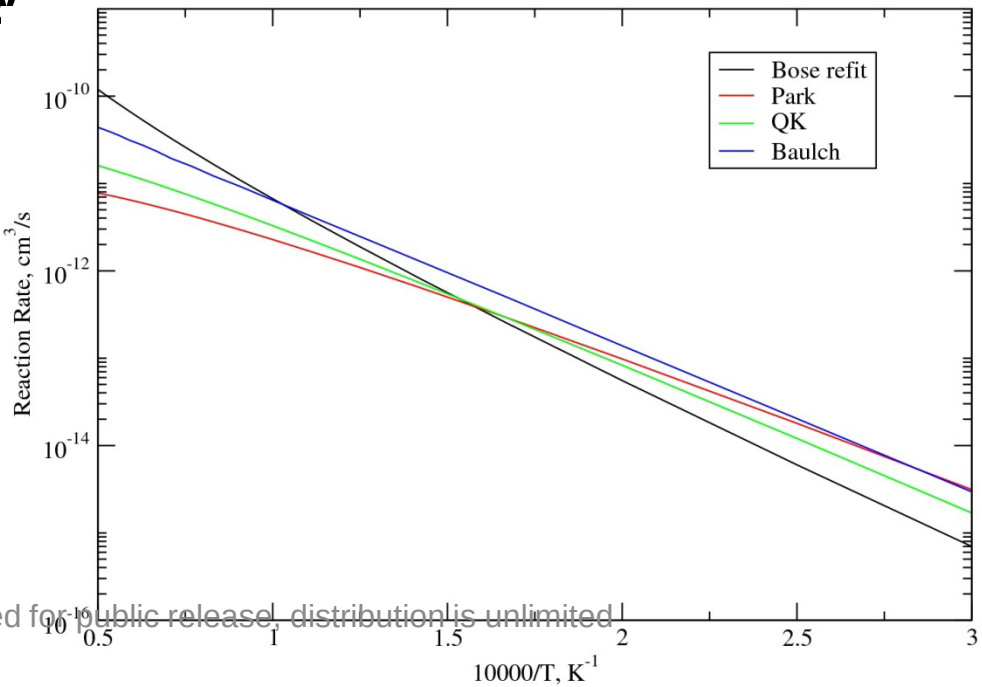
- For v=60, QCT has $\sigma_{diss} \geq \sigma_{total}$; QK very close to this
- TCE far underestimates the probability for very high v

- For flows with mainly low v populated, QK may be problematic



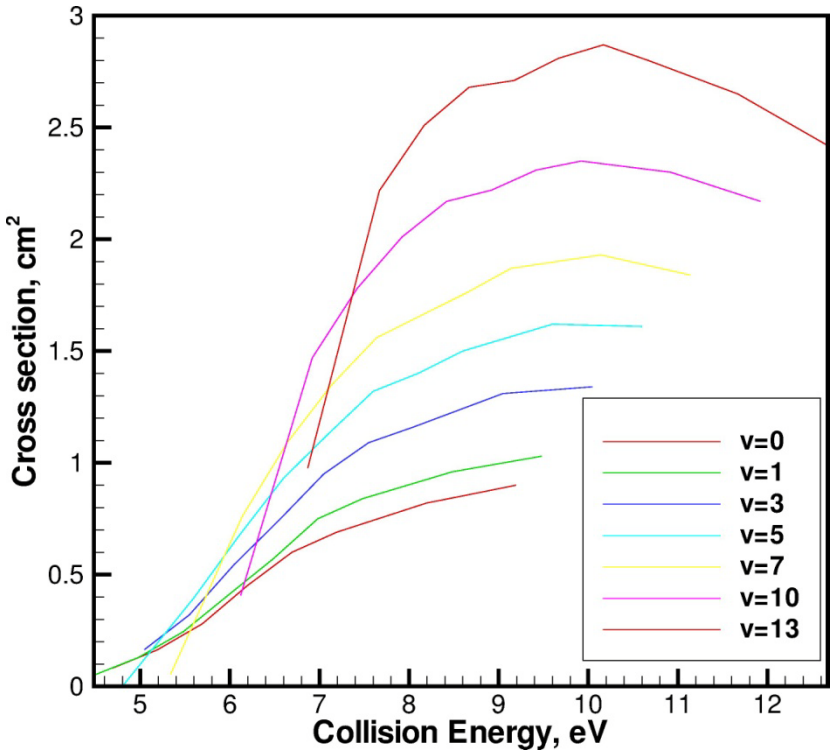
N_2+O Exchange Reaction k(T)

- N_2+O -> NO + N QCT results from Bose and Candler, unpublished
- Plot of thermal reaction rate coefficients
- TCE model uses published Arrhenius parameters as input and will match QCT k(T) by definition
- QK model uses no adjustable parameters and matches QCT (and expt) k(T) reasonably



N_2+O Exchange Reaction

- **This (and many other) exchange reactions have no strong vibrational favoring**

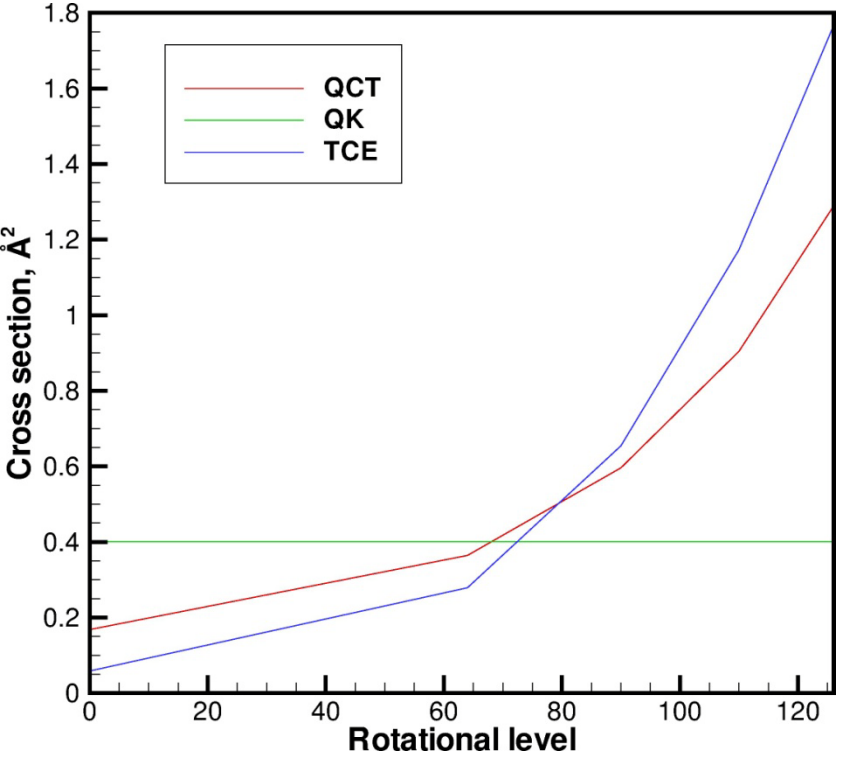


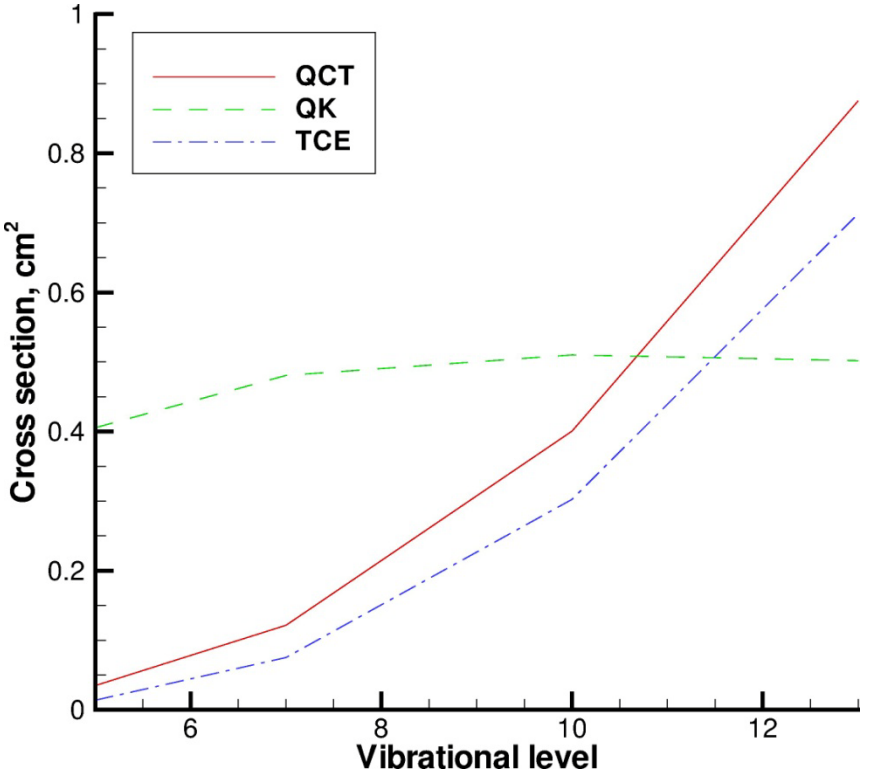
QCT cross sections at same E_c show ~3x difference in σ

Lends itself more readily to a simplified DSMC model

N_2+O Exchange Reaction

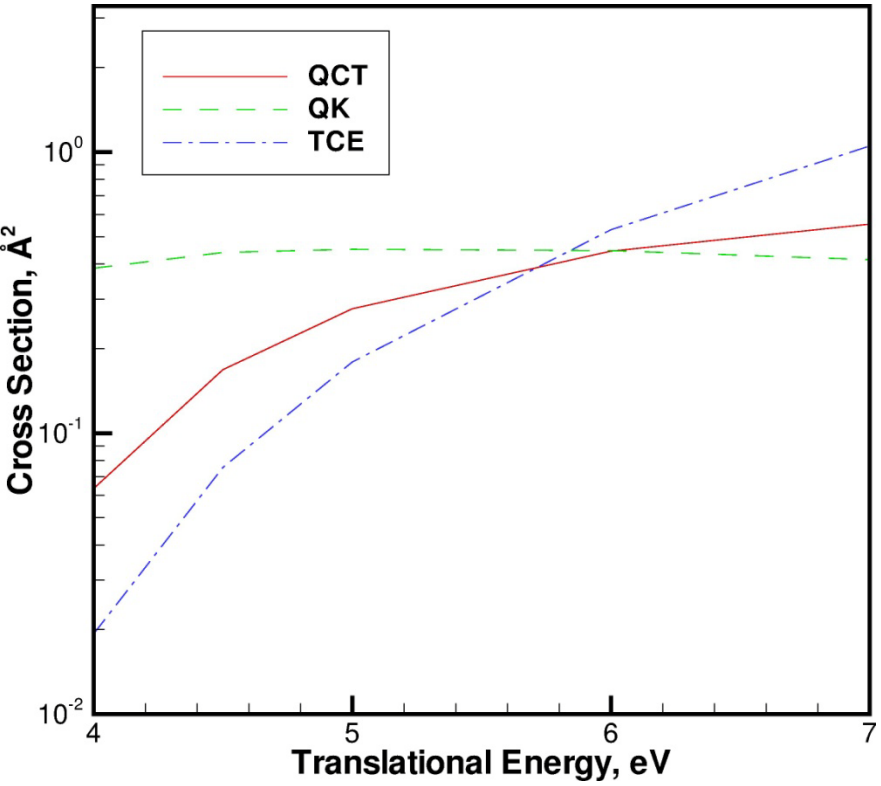
- **Overall shape of σ(E) much better represented by TCE model**

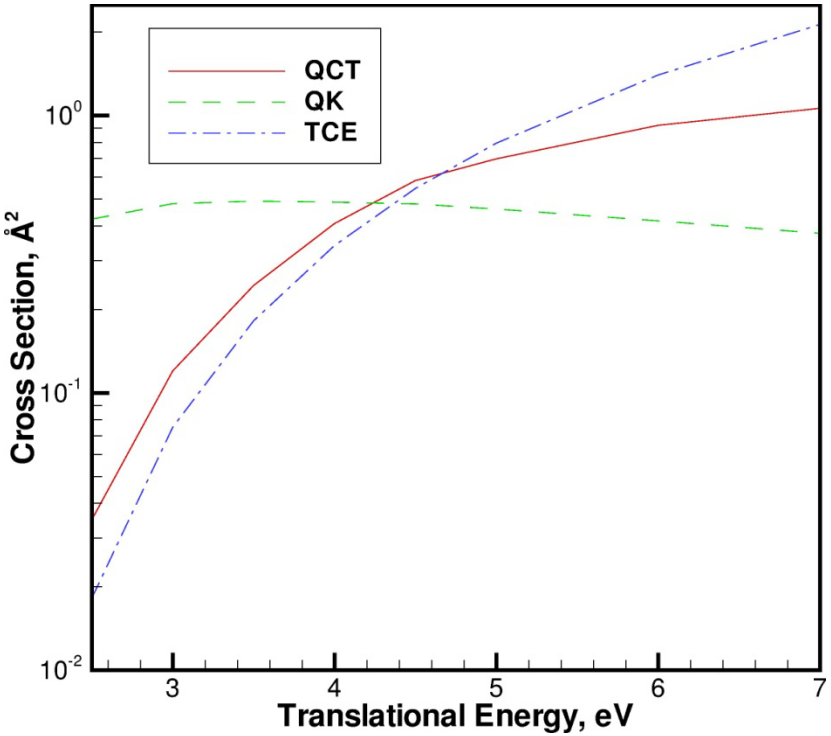




N_2+O Exchange Reaction

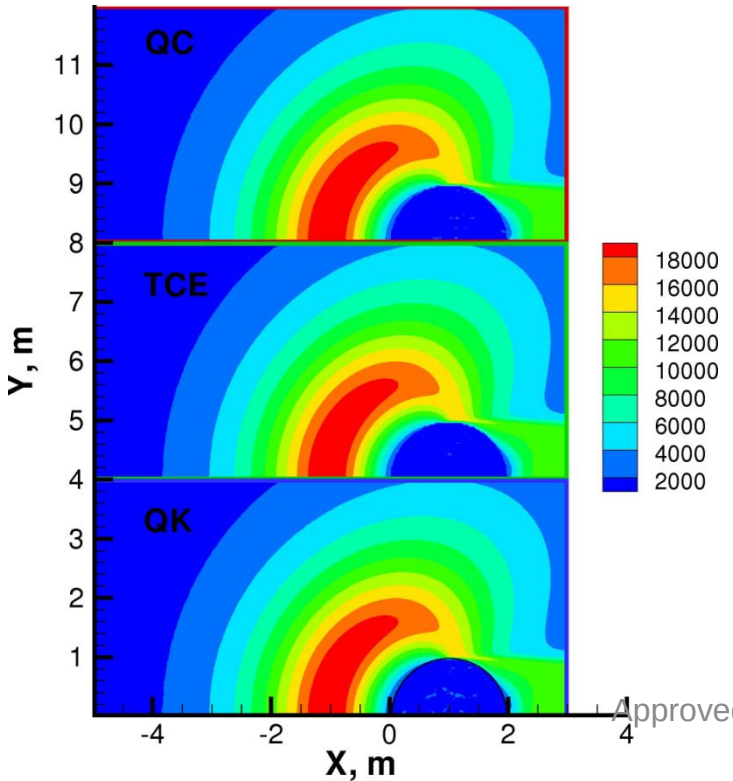
- **Overall shape of σ(E) much better represented by TCE model, v=0 and v=5 examples (J=0)**

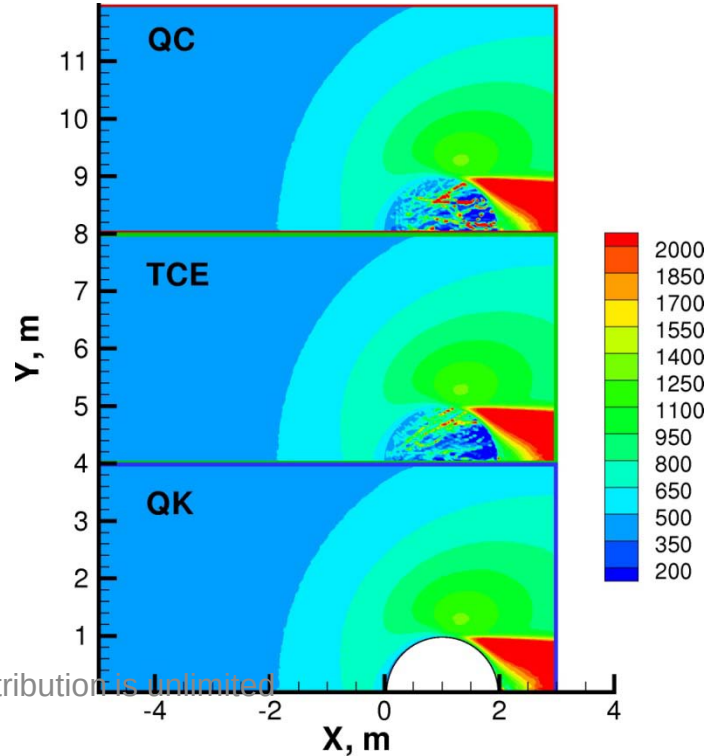




Sensitivity of Flowfield Results to N2+O reaction model

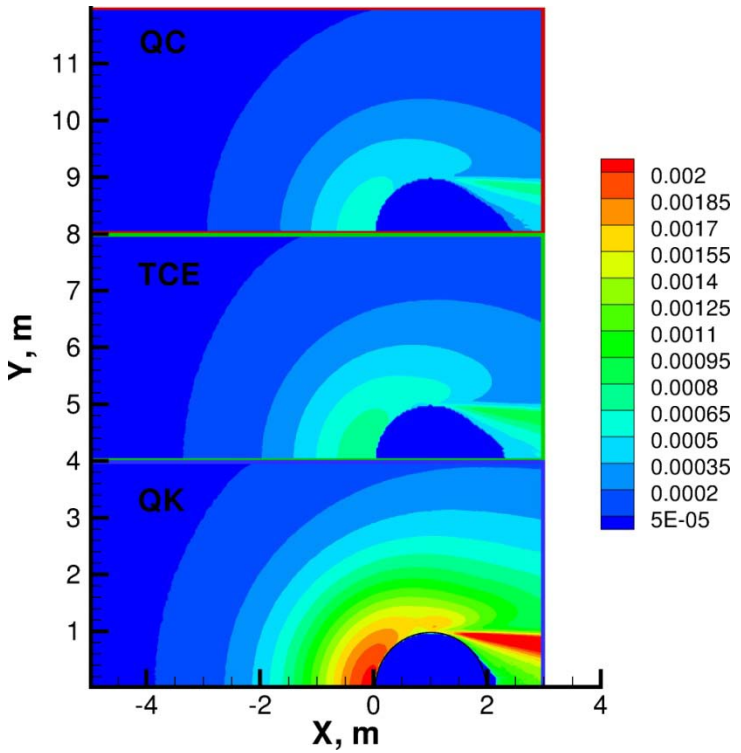
- **Simple axisymmetric flow over cylinder, 8 km/s, 120 km (fractions of N2, O?) nearly single-collision**
- **QCT cross sections were used in one run as look-up table with interpolation for comparison**





Sensitivity of Flowfield Results

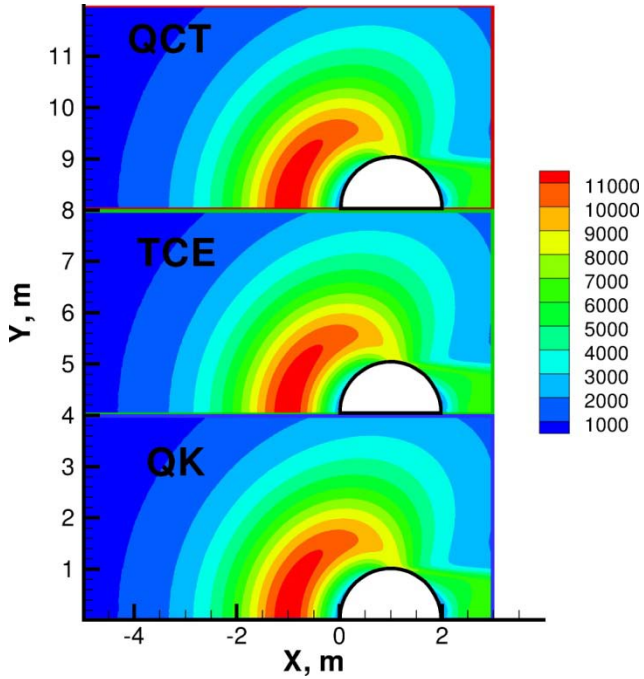
- **NO product mole fraction, 8 km/s**



- **Conclusion: As indicated by σ plot, QK model significantly overpredicts reaction probability near threshold**
- **QK NO fraction is 3x high**

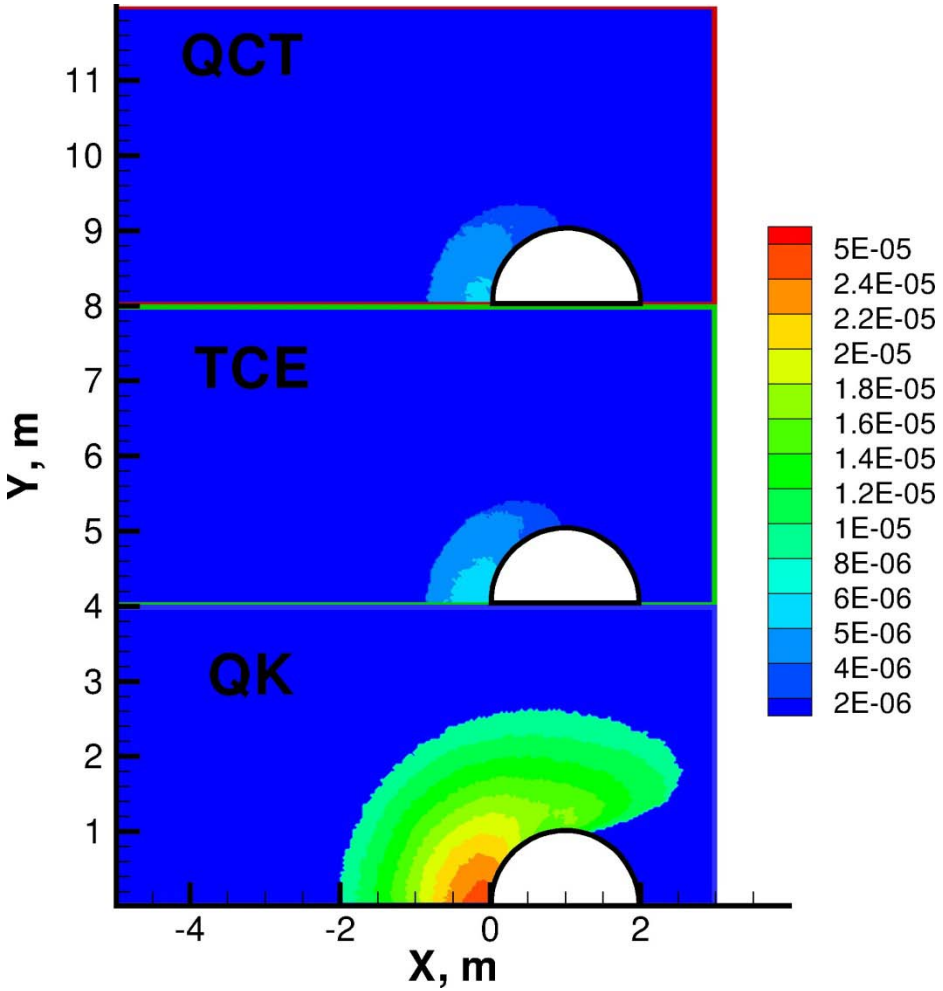
Sensitivity of Flowfield Results to N2+O reaction model

- **Simple axisymmetric flow over cylinder, 6 km/s, 120 km (fractions of N2, O?) nearly single-collision**



Sensitivity of Flowfield Results

- **NO product mole fraction, 6 km/s**



Conclusion: As indicated by σ plot, QK model significantly overpredicts reaction probability near threshold

Summary and Recommendations

- **Present results are complementary to previous publications on QK model, focusing on noneq aspects**
- **for strongly nonequilibrium flows, the probability of reaction is sensitive to the shape of the energy-dependent cross section; TCE more realistic than QK model in this respect**
- **Possibly explore gaining the best of both?**